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Superfund

Superfund Chemical Data Matrix

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SECTION 1
INTRODUCTION

The Superfund Chemical Data Matrix (SCDM) is a source for factor values and benchmark values applied when evaluating potential National Priorities List (NPL) sites using the Hazard Ranking System (HRS; 40 CFR Part 300, 55 *FR* 51583). The HRS assigns factor values for toxicity, gas migration potential, gas and ground water mobility, surface water persistence, and bioaccumulation potential based on the physical, chemical, and radiological properties of Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) hazardous substances present at a site. Hazardous substances, as defined for HRS purposes, are CERCLA hazardous substances plus CERCLA pollutants and contaminants. The HRS also assigns extra weight to targets with exposure levels to hazardous substances that are at or above benchmarks. These benchmarks include both risk-based screening concentrations and concentrations specified in regulatory limits for the hazardous substances present at a site for a particular migration pathway.

SCDM contains HRS factor values and benchmarks for hazardous substances that are frequently found at sites evaluated using the HRS, as well as the physical, chemical, and radiological data used to calculate those values. The raw data in SCDM are taken directly from literature sources or other databases or are calculated. HRS rules are then applied to the raw data to determine a factor value or benchmark.

Section 2 of this document explains how data are selected for inclusion in SCDM. Section 3 describes how some types of data (i.e., volatilization half-lives, distribution coefficients, and screening concentrations) are internally calculated using data in SCDM and methodologies from published literature or regulatory guidance documents. Section 4 describes how SCDM data, HRS factor values, and benchmark values are presented. The factor values and benchmark values are listed, substance by substance, in Appendix A. Appendix B-1 contains the HRS factor values and benchmark tables (organized by pathway) for nonradiological hazardous substances. Appendix B-2 contains similar tables for radionuclides, and Appendix C contains a cross-reference index of substance name synonyms.

1.1 DEFINITIONS

In addition to the definitions found in Section 1.1 of the HRS (55 *FR* 51585-51587), the following definitions are used in this document:

- **Cancer Risk Screening Concentrations**: Substance-specific intake concentrations that are based on a cancer slope factor and on estimates of a daily exposure level of a

substance. They are used in the HRS as benchmarks in evaluating target populations actually exposed to carcinogenic substances (see also the definitions of “Slope Factor” and “Screening Concentration” in Section 1.1 of the HRS).

- **Reference Dose Screening Concentrations**: Substance-specific intake concentrations that are based on a noncancer reference dose (RfD) and estimates of a daily exposure level of a substance. They are used in the HRS as benchmarks in evaluating target populations actually exposed to noncarcinogenic substances (see also the definitions of “Reference Dose” and “Screening Concentration” in Section 1.1 of the HRS).

SECTION 2

SUPERFUND CHEMICAL DATA MATRIX DATA SELECTION METHODOLOGY

This section describes how the data available in specified literature sources and regulatory guidance documents are selected for inclusion in SCDM. Section 2.1 describes how to resolve ambiguities that arise in determining whether particular values apply to particular hazardous substances. Sections 2.2 through 2.9 specify the references used to obtain the data for SCDM and the methodologies used to extract the data. The criteria described in these sections were developed based on the type and quality of data available in the current SCDM references; they are not intended to apply to all data in general. As different compilations of data become available, different criteria may be considered.

2.1 HAZARDOUS SUBSTANCE IDENTITIES AND SCDM PROTOCOLS

Compiling data for SCDM requires determining which data reasonably apply to a hazardous substance. Data in the references cited in Sections 2.2 through 2.9 are sometimes available for classes and mixtures of hazardous substances, but not for the individual substances that make up that mixture. Thus, there may be questions concerning whether the hazardous substance identities in the references match the hazardous substance identities in SCDM. This section describes how ambiguities in assigning particular values to members of classes of hazardous substances in SCDM have been resolved.

SCDM contains generic values for the following classes of compounds (for chromium and chlordane, these generic values are used only when the specific oxidation state or isomer concentration is not adequately known):

- chromium (III and VI oxidation states)
- arsenic (III and V oxidation states)
- mercury (elemental and inorganic compounds)
- polychlorinated biphenyls (PCBs) (various congeners and Arochlors)
- endosulfans (I and II)
- chlordane (α and γ).

In general, if any member of these classes is present at a hazardous substance site, it is assumed that the most toxic, most persistent, or most bioaccumulative member of the class is present. In other words, from among the data given in the specified references for members of these classes,

SCDM contains those data resulting in the greatest HRS factor values (e.g., lowest LD_{50}, longest half-life, greatest bioaccumulation factor).

For chromium, if the oxidation state is known, the generic values are not used. For arsenic, SCDM contains data for the more mobile and toxic arsenic III species. For mercury, SCDM contains data for elemental and inorganic species. The oral RfD is for mercuric chloride and the inhalation RfD is for elemental mercury vapor. Vapor pressure and Henry's law constant are for the elemental form, while the distribution coefficient is for the (+2) species.

PCBs are represented solely as a class of compounds in SCDM, with a single value used regardless of the mixture of compounds identified at a site. For PCBs, chemical properties in SCDM are based on Arochlor 1254, which results in the most conservative bioaccumulation/ human food chain-based factor values for this group of compounds. Although the endosulfans I and II can be distinguished analytically, no data for either isomer by itself are available in the designated sources. All data in SCDM represent a mixture of endosulfan isomers. SCDM contains some data for the α and γ isomers of chlordane, but, for the most part, values represent a mixture of the isomers.

For the following classes of compounds, SCDM contains values for individual substances:

- dichlorobenzenes
- dinitrotoluenes
- hexachlorocyclohexanes
- xylenes.

If no data can be found in the specified references for an individual substance in the class but data are available for the generic class, SCDM assigns the generic value to that substance. These classes are all relatively small sets of isomers, which are likely to occur as mixtures. Furthermore, these classes are well defined in the sense that the generic class (e.g., xylenes) almost always refers to a mixture of all members of the class (*o*-, *m*-, and *p*-xylene). The expected similarity in chemical behavior for members of each class, as well as the likelihood that they will occur as mixtures, makes using data from mixtures reasonable.

SCDM also defines another class of compounds containing the following polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans:

- 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD)
- 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin
- 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin
- 1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin
- 1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin

- 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin
- 2,3,7,8-tetrachlorodibenzofuran
- 1,2,3,7,8-pentachlorodibenzofuran
- 2,3,4,7,8-pentachlorodibenzofuran
- 1,2,3,4,7,8-hexachlorodibenzofuran
- 1,2,3,6,7,8-hexachlorodibenzofuran
- 1,2,3,7,8,9-hexachlorodibenzofuran
- 2,3,4,6,7,8-hexachlorodibenzofuran
- 1,2,3,4,6,7,8-heptachlorodibenzofuran
- 1,2,3,4,6,7,9-heptachlorodibenzofuran.

SCDM contains the cancer slope factor for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) from the Health Effects Assessment Summary Tables (HEAST) (EPA, 1995d). For all other dioxins and dibenzofurans, the cancer slope for TCDD is multiplied by the *toxicity equivalence factor* (TEF) for each substance to give an estimated slope factor that is entered into SCDM for that substance. TEF values are obtained from Section 3, Table 2 of EPA's *Interim Procedures for Estimating Risks Associated with Mixtures of Chlorinated Dibenzo*-p-*Dioxins and Dibenzofurans (CDDs and CDFs) and 1989 Update*, (1989a, p. 12). All members of this class are assigned the weight of evidence for TCDD (B2).

For cadmium, the Integrated Risk Information System (IRIS) contains two RfD values: one for drinking water and one for dietary exposure. Since SCDM calculates RfD-based screening concentrations for both drinking water and dietary exposure, and only one RfD per substance can be entered into SCDM, SCDM uses the more conservative drinking water RfD for cadmium.

The HRS specifies that a human toxicity factor of 10,000 be assigned to asbestos and lead compounds. SCDM does this automatically within the data manager's computer code.

2.2 TOXICITY INFORMATION

2.2.1 Reference Dose (RfD)—Oral, Inhalation

SCDM uses data from the following references (listed in order of preference) for oral and inhalation RfD:

1. U.S. Environmental Protection Agency (EPA). 1996a. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH.

2. U.S. Environmental Protection Agency (EPA). 1995d. *Health Effects Assessment Summary Tables (HEAST)*. EPA 5401R-95-036. Office of Research and Development, Washington, DC. NTIS PB95-921199.

SCDM prefers IRIS data over HEAST data. Inhalation data in IRIS are given as reference concentrations (RfCs) equivalent to dose rather than RfDs. RfCs are converted to RfDs by the following equation:

$$RfD_{inhal} = \frac{RfC \times IR \times AR}{BW \times 100} \quad (1)$$

where:

RfC = Reference concentration in air (mg/m^3)
IR = Inhalation rate (20 m^3/day)
AR = Absorption rate (%)
BW = Adult body weight (70 kg).

Using the default exposure assumptions listed above, Equation (1) may be simplified as:

$$RfD_{inhal}\ mg/kg\text{-}day = RfC_{inhal} \times AR \times 2.857 \times 10^{-3}\ . \quad (2)$$

Equation (2) is used to convert RfCs to RfDs for use in SCDM. If IRIS or HEAST does not provide an absorption rate, it is assumed to be 100 percent; this is consistent with the convention described in HEAST.

SCDM also contains interim or provisional reference dose values for certain hazardous substances for use in the Superfund site assessment program for compounds that do not have values in IRIS or HEAST. These values are identified by their datafile source, LIVECHEM, with data sources described in the LIVECHEM datafile comment field (not displayed on screen). Sources of human toxicity data in LIVECHEM are also given in:

Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response. Washington, DC.

2.2.2 LD_{50}—Oral, Dermal

SCDM uses data from the following references (listed in order of preference) for oral and dermal LD_{50}:

1. C-E Environmental, Inc. 1990. *The Identification of Health Effects Data for Chemicals Contained in the Clean Air Act Amendments: Final Report to Dr. John Vanderburg*. U.S. Environmental Protection Agency, Research Triangle Park, NC.

2. American Conference of Governmental Industrial Hygienists (ACGIH). 1991. *Documentation of the Threshold Limit Value and Biological Exposure Indices*. ACGIH, Cincinnati, OH.

3. National Institute for Occupational Safety and Health (NIOSH). 1995. *Registry of Toxic Effects of Chemical Substances (RTECS)*. NIOSH, Cincinnati, OH.

SCDM contains the lowest value for any mammalian species by the specified route of exposure (i.e., oral or dermal) in controlled dose studies in laboratory animals. Human lethality data (i.e., data from suicide and worker poisonings) are not used due to the associated inaccuracy of the dosage estimates. Data from former Eastern Bloc countries (e.g., former Soviet Union) are not used due to the typically poor data quality. Only data for exposure durations <24 hours are used. If an LD_{50} value is not given, SCDM uses an LD_{LO} value: (1) if it is for the same exposure route, (2) if it has an exposure <24 hours, and (3) if it is reasonable relative to the other values (e.g., relative to chronic values) given for that substance and exposure route.

2.2.3 LC_{50}—Inhalation

SCDM uses data from the following references (listed in order of preference) for inhalation LC_{50}:

1. American Conference of Governmental Industrial Hygienists (ACGIH). 1991. *Documentation of the Threshold Limit Value and Biological Exposure Indices*. ACGIH, Cincinnati, OH.

2. National Institute for Occupational Safety and Health (NIOSH). 1995. *Registry of Toxic Effects of Chemical Substances (RTECS)*. NIOSH, Cincinnati, OH.

SCDM contains the lowest value for any mammalian species by inhalation in controlled dose studies in laboratory animals. Human lethality data (i.e., data from suicide and worker poisonings) are not used due to the associated inaccuracy of the dosage estimates. Data from former Eastern Bloc countries (e.g., former Soviet Union) are not used due to the typically poor data quality. Only data for exposure durations <24 hours are used. If an LC_{50} value is not given, SCDM uses an LC_{LO} value: (1) if it is for the same exposure route, (2) if it has an exposure <24 hours, and (3) if it is reasonable relative to the other values (e.g., relative to chronic values) given for that substance and exposure route.

2.3 CARCINOGENICITY INFORMATION

2.3.1 Cancer Slope Factor (SF) and Weight of Evidence—Oral, Inhalation

SCDM uses data from the following references (listed in order of preference) for oral and inhalation cancer slope factors and the associated weights of evidence:

1. U.S. Environmental Protection Agency (EPA). 1996a. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH.

2. U.S. Environmental Protection Agency (EPA). 1995d. *Health Effects Assessment Summary Tables (HEAST)*. EPA-540/R-95-036. Office of Research and Development, Washington, DC. NTIS PB95-921199.

SCDM prefers IRIS values for nonradioactive hazardous substances over HEAST values. For radioactive hazardous substances, SCDM contains values from HEAST.

Data in IRIS for inhalation are given as unit risk factors (URFs), which are related to cancer slope factors by the following equation (used for nonradionuclides only):

$$SF_{inhal} = \frac{URF \times BW \times CF \times 100}{IR \times AR} \quad (3)$$

where:

SF = Cancer slope factor $(mg/kg\text{-}day)^{-1}$
URF = Unit risk factor $(\mu g/m^3)^{-1}$
BW = Adult body weight (70 kg)
CF = Conversion factor (1,000 µg/mg)
IR = Inhalation rate (20 m^3/day)
AR = Absorption rate (%).

Using the assumptions listed above reduces Equation (3) to the following equation:

$$SF_{inhal}\ (mg/kg\text{-}day)^{-1} = \frac{URF \times 3.50 \times 10^5}{AR}\ . \quad (4)$$

Equation (4) is used to convert unit risk to cancer slope factors for use in SCDM. If IRIS or HEAST does not provide an absorption rate, it is assumed to be 100 percent; this is consistent with the convention described in HEAST.

SCDM uses the weight of evidence from the same reference that provides the corresponding slope factor. Typically, IRIS reports a single weight of evidence; this value is recorded separately as both the oral weight of evidence and the inhalation weight of evidence. In HEAST, there are usually two values listed, one for oral and one for inhalation. Usually these values are identical; SCDM records each value separately.

SCDM also contains interim or provisional cancer slope factors for certain hazardous substances for use in the Superfund site assessment program for compounds that do not have values in IRIS or HEAST. These values are identified by their datafile source, LIVECHEM, with data sources given in the LIVECHEM datafile comment field (not displayed on screen). Sources of human toxicity data in LIVECHEM are also given in:

Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

2.3.2 ED_{10} and Weight of Evidence—Oral, Inhalation

SCDM uses data from the following references (listed in order of preference) for oral and inhalation ED_{10} and the associated weights of evidence:

1. U.S. Environmental Protection Agency (EPA). 1988. *Methodology for Evaluating Potential Carcinogenicity in Support of Reportable Quantity Adjustments Pursuant to CERCLA Section 102* (EPA_ED10). Office of Health and Environmental Assessment, Washington, DC (EPA/600/8-89/053).

2. U.S. Environmental Protection Agency (EPA). 1986. *Superfund Public Health Evaluation Manual (SPHEM)*. Office of Emergency and Remedial Response, Washington, DC (EPA/540/1-86/060).

A single potency factor ($1/ED_{10}$) is reported for oral and inhalation exposure routes in EPA (1988). The reported value is the reciprocal of ED_{10}. Therefore, the oral and inhalation ED_{10} values contained in SCDM are calculated by taking the reciprocal of the potency factor (i.e., ED_{10} = 1/potency factor).

2.4 MOBILITY INFORMATION

2.4.1 Vapor Pressure

SCDM generally uses data from the following references (listed in order of preference) for vapor pressure:

1. U.S. Environmental Protection Agency (EPA). 1995c. FATE Database. Office of Research and Development, Athens, GA.

2. Syracuse Research Corporation (SRC). 1995. CHEMFATE Database. SRC, Syracuse, NY.

3. CHEMCALC values, calculated according to procedures in Lyman et al. (1990), as described in Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

4. GSC Corporation. 1990. CHEMEST Database. Developed for U.S. EPA Office of Pesticides and Toxic Substances, Washington, DC.

SCDM only uses measured values from the FATE database. If an estimated or calculated value is presented in FATE, that value is not used in SCDM. Within CHEMFATE, the recommended value is preferred. If more than one recommended value is available, SCDM uses the highest value. If a recommended value is not available, SCDM uses a value measured at 25 °C. If more than one value measured at 25 °C is available, SCDM uses the highest one. If values are not available for measurements at 25 °C, values determined within the range of 20 to 30 °C are used. If there is more than one value measured at the same temperature and none is recommended, SCDM uses the highest value. If no temperature is specified in CHEMFATE for all vapor pressure measurements for a substance, SCDM uses the highest value.

If vapor pressure values are not available in either FATE or CHEMFATE, the procedures described in Lyman et al. (1990) are used to calculate vapor pressure, which is entered in the CHEMCALC datafile. RTI (1996) describes the use of these procedures for specific hazardous substances found in SCDM. If these procedures are not applicable, a CHEMEST estimated value is used.

The above heirarchy is superseded by values in the LIVECHEM datafile when a value selected by the heirarchy is suspect or a measured value is not available in the SCDM data sources. For a particular chemical, suspect values are identified by comparison with other vapor pressure values in SCDM data sources or other sources of chemical property data. The

LIVECHEM datafile includes a comment field (not displayed onscreen by SCDM-DM) listing the source of each LIVECHEM value. RTI (1996) describes the selection of LIVECHEM values and documents their sources.

For nonmetallic substances, if vapor pressure is not available, a normal boiling point is obtained from the *Handbook of Chemistry and Physics* (Lide, 1994) and entered into BASEDATA. If a boiling point is not available from the handbook, a value from the Merck Index (Merck, 1989) is used. If the boiling point at 1 atmosphere (atm) is <25 °C, a default vapor pressure of 760 Torr is entered into LIVECHEM (i.e., the compound is assumed to be a gas at 25 °C).

If no vapor pressure is available for a substance and the normal boiling point is ≥25 °C, SCDM assumes that the substance is in a particulate rather than a gaseous form, and no default vapor pressure value is assigned. This assumption is made because the absence of a vapor pressure value often reflects an extremely low and difficult-to-measure (under standard conditions) value for nongaseous substances.

2.4.2 Henry's Law Constant

SCDM uses data from the following references (listed in order of preference) for Henry's law constant (HLC):

1. U.S. Environmental Protection Agency (EPA). 1995c. FATE Database. Office of Research and Development, Athens, GA.

2. Syracuse Research Corporation (SRC). 1995. CHEMFATE Database. SRC, Syracuse, NY.

3. CHEMCALC values, calculated according to procedures in Lyman et al. (1990) (no values available for June 1996 version).

4. GSC Corporation. 1990. CHEMEST Database. Developed for U.S. EPA Office of Pesticides and Toxic Substances, Washington, DC.

SCDM uses only measured values from the FATE database. If an estimated or calculated value is presented in FATE, that value is not used in SCDM. Within CHEMFATE, the recommended value is preferred. If more than one recommended value is available, SCDM uses the highest value. If a recommended value is not available, SCDM uses a value measured at 25 °C. If more than one value measured at 25 °C is available, SCDM uses the highest one. If values are not available for measurements at 25 °C, values determined within the range of 20 to 30 °C are used. If more than one value measured at the same temperature is available and none

is recommended, SCDM uses the highest value. If temperature is specified in CHEMFATE for all HLC measurements for a substance, SCDM uses the highest value.

If HLC values are not available in either FATE or CHEMFATE, the procedures described in Lyman et al. (1990) are used to calculate an HLC. If these procedures do not apply, a CHEMEST estimated value is used.

The above heirarchy is superseded by values in the LIVECHEM datafile when a value selected by the heirarchy is suspect or a measured value is not available in the SCDM data sources. For a particular chemical, suspect values are identified by comparison with other Henry's law values in SCDM data sources or other sources of chemical property data. The LIVECHEM datafile includes a comment field (not displayed on screen by SCDM-DM) listing the source of each LIVECHEM value. RTI (1996) describes the selection of LIVECHEM values and documents their sources.

2.4.3 Water Solubility—Nonmetallic Compounds

SCDM uses data from the following references (listed in order of preference) for water solubility for nonmetallic compounds:

1. U.S. Environmental Protection Agency (EPA). 1995c. FATE Database. Office of Research and Development, Athens, GA.

2. Syracuse Research Corporation (SRC). 1995. CHEMFATE Database. SRC, Syracuse, NY.

3. CHEMCALC values, calculated according to procedures in Lyman et al. (1990), as described in Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

4. GSC Corporation. 1990. CHEMEST Database. Developed for U.S. EPA Office of Pesticides and Toxic Substances, Washington, DC.

SCDM uses only measured values from the FATE database. If an estimated or calculated value is presented in FATE, that value is not used in SCDM. Within CHEMFATE, the recommended value is preferred. If more than one recommended value is available, SCDM uses the highest value. If a recommended value is not available, SCDM uses a value measured at 25 °C. If more than one value measured at 25 °C is available, SCDM uses the highest one. If values are not available for measurements at 25 °C, values determined within the range of 20 to 30 °C are used. If more than one value measured at the same temperature is available and none

is recommended, SCDM uses the highest value. If no temperature is specified in CHEMFATE for all water solubility measurements for a substance, SCDM uses the highest value.

If water solubility values are not available in either FATE or CHEMFATE, the procedures described in Lyman et al. (1990) are used to calculate water solubility. RTI (1996) describes the use of these procedures for specific hazardous substances found in SCDM. If these procedures do not apply, a CHEMEST estimated value is used.

The above heirarchy is superseded by values in the LIVECHEM datafile when a value selected by the heirarchy is suspect or a measured value is not available in the SCDM data sources. For a particular chemical, suspect values are identified by comparison with other water solubility values in SCDM data sources or other sources of chemical property data. The LIVECHEM datafile includes a comment field (not displayed onscreen by SCDM-DM) listing the source of each LIVECHEM value. RTI (1996) describes the selection of LIVECHEM values and documents their sources.

2.4.4 Water Solubility—Metals and Metalloids

SCDM uses data from the following references (in order of preference) for water solubility of metals and metalloid compounds:

1. Weast, R.C. 1981. *Handbook of Chemistry and Physics*. 62nd ed. CRC Press, Cleveland, OH. pp. B-73–B-166.

2. Dean, J.A. (Ed.). 1985. *Lange's Handbook of Chemistry*, 13th ed. McGraw-Hill, New York. pp. 5-7–5-12.

SCDM contains geometric mean water solubility values that are defined in the HRS as the geometric mean of the highest and the lowest water solubility values available for any inorganic compound containing the metal or metalloid. Highest and lowest compound solubility values were taken directly from Weast (1981), except for the following low-solubility compounds:

- copper (II) sulfide
- lead (II) sulfide
- mercury (II) sulfide
- nickel (II) sulfide
- silver (I) sulfide
- thallium (III) hydroxide
- thorium (IV) hydroxide
- uranyl hydroxide
- zinc (II) sulfide.

Solubility values for these compounds were calculated using the standard expression for the solubility product (K_{sp}) for each compound and the K_{sp} value taken from Dean (1985).

2.4.5 Soil/Water Distribution Coefficient (K_d)

SCDM uses data from the following references (listed in order of preference) for soil/water distribution coefficients (K_d) values for metals:

1. U.S. Envrionmental Protection Agency (EPA). 1996b. *Soil Screening Guidance: Technical Background Document*. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502.

2. Baes III, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. *A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides through Agriculture*. Oak Ridge National Laboratory, Oak Ridge, TN. ORNL-5786.

For metals, SCDM uses K_d values contained in EPA (1996b) that were estimated for the Soil Screening Guidance using the MINTEQ aqueous speciation geochemical model or, when the required thermodynamic data are not available in the MINTEQ databases, using empirical pH-dependent relationships developed by EPA's Office of Research and Development Laboratory in Athens, Georgia. Values corresponding to a typical subsurface pH (6.8) are used in SCDM. The derivation of these metal K_d values is described in EPA (1996b).

For organic hazardous substances, SCDM uses K_d values calculated using the following relationship between K_d and K_{oc}:

$$K_d = K_{oc} \times f_{oc} \quad (5)$$

where:

K_{oc} = Soil organic carbon/water partition coefficient (mL/g)
f_{oc} = Fraction of organic carbon in soil (g carbon/g soil).

The f_{oc} is assumed to be 0.002 g/g, which is typical of subsurface soils. This f_{oc} and the K_{oc} values used in SCDM are consistent with those used for the Soil Screening Guidance. SCDM datafiles (SSG_KD and RTI_ION) contain K_d values calculated from Soil Screening Guidance K_{oc} values for volatile organic compounds, certain chlorinated pesticides, and ionizing organic compounds. K_{oc} values for organic hazardous substances that ionize under subsurface pH conditions (i.e., pH = 4.9 to 8.0) are derived by applying a theoretical relationship that accounts for both the neutral and the ionized fractions of the compound. Values corresponding to a typical subsurface pH (pH = 6.8) are used in SCDM. The methodology used to develop these K_{oc} values is described in *Soil Screening Guidance: Technical Background Document*. K_d values for other organic compounds are calculated directly from Log K_{ow} values in SCDM, as described in

Section 3.2. RTI (1996) provides additional detail on the selection of soil/water distribution coefficients for organic compounds in SCDM.

2.5 PERSISTENCE INFORMATION

2.5.1 Hydrolysis, Biodegradation, and Photolysis Half-Lives

SCDM uses data from the following references (listed in order of preference) for hydrolysis, biodegradation, and photolysis half-lives:

1. U.S. Environmental Protection Agency (EPA). 1995c. FATE Database. Office of Research and Development, Athens, GA.

2. Howard, P.H., W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. *Handbook of Environmental Degradation Rates* (FATERATE). Lewis Publishers/CRC Press, Boca Raton, FL.

3. Syracuse Research Corporation (SRC). 1995. CHEMFATE Database. SRC, Syracuse, NY.

SCDM only uses measured values from the FATE Database. If estimated or calculated values are presented in FATE, those values are not used in SCDM. SCDM only uses values listed as "first-order" in Howard et al. (1991). If high and low values are given, the highest values are used. Within CHEMFATE, the recommended values are preferred. If more than one recommended value is available, the highest is selected. If a recommended value is not available, SCDM uses a value measured at 25 °C. If more than one value measured at 25 °C is available, the highest is selected. If values are not available for measurements at 25 °C, values determined within the range of 20 to 30 °C are used. If there is more than one value measured at the same temperature and none is recommended, SCDM uses the highest value. If no half-life value is provided in CHEMFATE, the half-life used in SCDM is calculated based on the percent change over time by assuming a first-order rate law.

2.5.2 Radioactive Half-Life

SCDM uses data from the following reference for radioactive half-life:

International Commission on Radiological Protection (ICRP). 1983. *Radionuclide Transformations: Energy and Intensity of Emissions*. ICRP Publication No. 38. Pergamon Press, New York.

If more than one value is given for a single decay mode, SCDM uses the highest value. If values are given for more than one decay mode, the half-life of the isotope is computed from the values for all decay modes according to the following formula:

$$t_{1/2} = 1/(1/t_1 + 1/t_2 \ldots + 1/t_n) \quad (6)$$

where:

$t_{1/2}$ = Half-life of the isotope
t_1 = Value given for the first decay mode
t_2 = Value given for the second decay mode
t_n = Value given for the n-th decay mode.

2.6 BIOACCUMULATION POTENTIAL INFORMATION

2.6.1 Bioconcentration Factor—Freshwater, Saltwater

SCDM uses data from the following references (listed in order of preference) for freshwater and saltwater bioconcentration factors (BCFs):

1. Versar, Inc. 1990. *Issue Paper: Bioaccumulation Potential Based on Ambient Water Quality Criteria Documents* (VER_BCF). Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC. Contract No. 68-W8-0098.

2. U.S. Environmental Protection Agency (EPA). 1995a. Aquatic Information Retrieval (AQUIRE) Database. Environmental Research Laboratory, Duluth, MN.

SCDM contains the highest measured value from the Versar (1990) document in preference to an estimated value from the same document. If no value is reported in Versar (1990), the highest value from AQUIRE is used. All values where no environment (i.e., saltwater or freshwater) is given but that list NaCl as a control are considered as freshwater values.

SCDM uses the highest value from the following aquatic organisms to establish human food chain threat BCF values (this list includes only aquatic human food chain organisms in the cited references and is not meant to be a complete list of aquatic human food chain organisms):

- American or Virginia oyster
- Asiatic clam
- Atlantic salmon
- Atlantic silverside
- black crappie
- black bullhead

- black mussel
- blue crab
- bluegill
- brook trout
- brown trout
- channel catfish
- clam
- common bay mussel
- common mirror colored carp
- common shrimp
- crayfish
- dungeness or edible crab
- giant gourami
- gulf toadfish
- kiyi
- lake trout (siscowet)
- lake whitefish
- mangrove snapper
- Manila littleneck clam
- mussel
- northern pike
- northern anchovy
- pilchard sardine
- pinfish
- pink salmon
- rainbow trout
- red swamp crayfish
- rock bass
- sauger
- shore crab
- spot
- striped bass
- striped mullet
- swan mussel
- tong sole
- topmouth gudgeon (golden shiner)
- white mullet
- white sand mussel

Nonhuman food chain aquatic organisms are not used for the food chain BCF. The highest value from *any* aquatic organism mentioned in each reference is used to establish environmental threat BCF values, using the same order of preference described above.

2.6.2 Octanol/Water Partition Coefficient (Log K_{ow})

For *n*-octanol/water partition coefficient (K_{ow}), SCDM uses Log K_{ow} (also referred to as Log P) data from the following references (listed in order of preference):

1. Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

2. U.S. Environmental Protection Agency (EPA). 1995c. FATE Database. Office of Research and Development, Athens, GA.

3. Syracuse Research Corporation (SRC). 1995. CHEMFATE Database. SRC, Syracuse, NY.

4. GSC Corporation. 1990. CHEMEST Database. Developed for U.S. EPA Office of Pesticides and Toxic Substances, Washington, DC.

Most of the chemicals in SCDM are addressed in RTI (1996). Many of these values were selected by EPA's Office of Research and Development in Athens, Georgia (ORD-Athens), from an extensive list of measured values compiled by RTI and values calculated by ORD-Athens using the SPARC and CLOGP computer programs. Values not selected by ORD-Athens were selected by RTI from a compilation of measured values. Compilation and selection procedures are described in RTI (1996). SCDM only uses measured values from the FATE database. If estimated or calculated values are presented in FATE, those values are not used in SCDM. SCDM uses only recommended values from the CHEMFATE Database. CHEMEST estimated Log K_{ow} values are used if values are not available from the other data sources.

2.7 ECOTOXICITY PARAMETERS

2.7.1 Acute and Chronic Freshwater and Saltwater Criteria

SCDM uses data from the following reference for acute and chronic freshwater and saltwater criteria:

U.S. Environmental Protection Agency (EPA). 1995e. *Water Quality Criteria-Draft (the Silver Book*). Office of Water, Washington, DC.

SCDM uses only values that are specifically stated as criteria. At this time, no Ambient Aquatic Life Advisory Concentrations (AALACs) have been specified.

2.7.2 LC_{50}—Freshwater, Saltwater

SCDM uses data from the following reference for freshwater and saltwater LC_{50} values:

U.S. Environmental Protection Agency (EPA). 1995a. Aquatic Information Retrieval (AQUIRE) Database. Environmental Research Laboratory, Duluth, MN.

SCDM uses the lowest, acute LC_{50} value found for any aquatic organism in the specified environment with an acute exposure duration of >1 day and ≤4 days. All LC_{50} values where no environment is given but that use NaCl as a control are considered as freshwater LC_{50} values. When no durations or environments are given, LC_{50} values are not entered into SCDM.

2.8 REGULATORY BENCHMARKS

The HRS assigns extra weight to targets with exposure levels to hazardous substances that are at or above benchmark values. This section describes the sources for certain regulatory limits that the HRS uses as health-based or ecological-based benchmarks.

2.8.1 National Ambient Air Quality Standards

SCDM uses data from the following reference for National Ambient Air Quality Standards (NAAQS):

40 CFR Part 50. 1994. National Ambient Air Quality Standards.

2.8.2 National Emissions Standards for Hazardous Air Pollutants

SCDM uses the following reference for National Emission Standards for Hazardous Air Pollutants (NESHAP):

40 CFR Part 61. 1994. National Emission Standards for Hazardous Air Pollutants.

SCDM uses only values that are reported in ambient concentration units ($\mu g/m^3$).

2.8.3 Maximum Contaminant Levels and Maximum Contaminant Level Goals

SCDM uses the following reference for Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs):

U.S. Environmental Protection Agency (EPA). 1995b. *Drinking Water Regulations and Health Advisories*. Office of Water, Washington, DC.

SCDM uses only MCLs that are reported in units of concentration (mg/L or µg/L). SCDM does not contain MCLs for total trihalomethanes (bromoform + bromodichloromethane + chloroform + dibromochloromethane), asbestos, radium isotopes, gross α-particle activity, or β-particle plus photon radioactivity.

SCDM uses only nonzero MCLGs that are reported in units of concentration (mg/L or µg/L). For substances where multiple values are listed due to lack of consensus on appropriate carcinogen class, SCDM contains the lowest number. For substances where both MCLs and MCLGs are reported but are different, SCDM selects the MCLG as the lower of the two values (55 *FR* 51593).

2.8.4 FDA Action Level

SCDM uses the following references (listed in order of preference) for Food and Drug Administration (FDA) Action Levels:

1. U.S. Food and Drug Administration. 1994. *Changes in Action Levels, Addendum to the 1992 Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed*. Center for Food Safety and Applied Nutrition, Washington, DC.

2. U.S. Food and Drug Administration. 1992. *Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed*. Center for Food Safety and Applied Nutrition, Washington, DC.

SCDM contains FDA Action Levels for fish and shellfish only.

2.8.5 Uranium Mill Tailings Radiation Control Act Standards

SCDM uses the following reference for Uranium Mill Tailings Radiation Control Act (UMTRCA) standards:

40 CFR Part 192. 1994. Uranium Mill Tailings Radiation Control Act Standards.

2.8.6 Ecological Based Benchmarks

The Ambient Water Quality Criteria and the Ambient Aquatic Life Advisory Concentrations discussed in Section 2.7.1 are also used to assign the ecological-based benchmarks.

2.9 OTHER CHEMICAL DATA

SCDM contains other chemical data and information that are not contained in the 28 data-files previously discussed. This information is contained in the BASEDATA file.

2.9.1 Physical Properties

SCDM uses data from the following references (listed in order of preference) for chemical formula, molecular weight, density, boiling point, and melting point:

1. Lide, D.R. (Ed.). 1994. *CRC Handbook of Chemistry and Physics*. 75th ed. CRC Press, Boca Raton, FL.

2. Merck. 1989. *The Merck Index*. 11th Edition. S. Budavari, Ed. Merck & Co., Inc., Rahway, NJ.

Data are extracted directly from *Section 3. Physical Constants of Organic Compounds* and *Section 4. Properties of the Elements and Inorganic Compounds* in the CRC Handbook. If data are unavailable in the CRC Handbook, or if the conditions of the experiment are not appropriate

to standard conditions (e.g., temperature is not in the range of 20 to 30 °C), data from the Merck Index are used.

Density values are extracted (preferably in g/mL or g/cc) along with the temperature at which the density was measured (preferably Celsius, or °C). If multiple values are available for density, the value measured closest to 25 °C is selected.

Boiling point and melting point are extracted (preferably in °C) along with the pressure at which boiling point was measured. Note that tests to determine the melting point are usually performed at the same pressure as the boiling point tests. If multiple values are available, the value measured closest to 1 atm (760 Torr or 760 mm Hg) is selected.

2.9.2 Logical Fields

SCDM uses four logical (or boolean yes/no) flags to classify substances that are entered into BASEDATA.

- Organic Substance ("Organic")—"Y" indicates that the substance is organic, and "N" indicates an inorganic substance. This flag is used to determine factor values for ground water mobility and bioaccumulation potential.

- Metal-Containing Substance ("Metal Contain")—"Y" indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. "N" indicates that the substance is not, or does not contain, a metal or metalloid. This flag is used to determine factor values for ground water mobility and surface water persistence.

- Radioactive Isotope ("Radionuclide")—"Y" indicates that the substance is a radionuclide or radioactive isotope, and "N" indicates that it is not. A substance in SCDM cannot be both a radioactive element and a radioactive isotope. This flag is used to determine factor values for human toxicity, ecosystem toxicity, and surface water persistence.

- Radioactive Element ("Rad. Element")—"Y" indicates that the substance is a radioactive element, and "N" indicates that it is not. This flag determines whether or not the HRS factors and benchmarks are printed in Appendix A.

2.9.3 Substitution Classes

SCDM contains fields for three substitution classes: toxicity, ground water mobility, and other data. For a particular chemical, a parent CAS number can be entered for any of these three substitution classes and SCDM automatically copies the relevant data from the parent chemical to the chemical of interest. Toxicity class data include all toxicity and benchmark data used to

determine human or ecotoxicity factor values. Ground water mobility class data include water solubility, geometric mean water solubility, and soil/water distribution coefficient (K_d). "Other" class data include hydrolysis, biodegredation, photolysis, and volatilization half-lives, as well as BCF and Log K_{ow}.

Currently two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for the ground water mobility class with the elemental metal as the class parent. Radioactive isotopes may inherit data from their primary radioactive element for the ground water and "other" classes.

SECTION 3

CALCULATIONS IN SUPERFUND CHEMICAL DATA MATRIX

3.1 VOLATILIZATION HALF-LIFE

SCDM estimates volatilization half-life in surface water for organic substances using Equation 15-12 from Thomas (1990). In this method, the volatilization half-life ($\tau_{1/2}$) can be expressed as follows,

$$\tau_{1/2} = \frac{Z \times \ln 2}{K_L \text{ hr}} \tag{7}$$

where:

Z = Mean water body depth (cm)
K_L = Overall liquid-phase mass transfer coefficient.

The following expression gives the overall liquid-phase mass transfer coefficient:

$$K_L = \frac{(H/RT)k_g \times k_1}{(H/RT)k_g + k_1} \text{ cm/hr} \tag{8}$$

where:

H = Henry's law constant (atm·m^3/mol)
R = Universal gas constant (8.2 × 10^{-5} atm·m^3/mol·K)
T = Temperature (K ;°C + 273)
k_g = Gas-phase exchange coefficient
k_l = Liquid-phase exchange coefficient.

The gas-phase exchange coefficient expression depends on the molecular weight (MW) of the compound. If MW is <65 g/mol, the following equation is used:

$$k_g = 3{,}000 \times (18/MW)^{1/2} \text{ cm/hr} . \tag{9}$$

If MW is ≥65 g/mol, the following equation is used:

$$k_g = 1{,}137.5 \times (V_{wind} + V_{curr}) \times (18/MW)^{1/2} \text{ cm/hr} \quad (10)$$

where:

V_{wind} = Wind velocity (m/sec)
V_{curr} = Current velocity (m/sec).

The liquid-phase exchange coefficient expression also depends on the molecular weight of the compound. If MW is <65 g/mol, the following equation is used:

$$k_1 = 20 \times (44/MW)^{1/2} \text{ cm/hr} . \quad (11)$$

If MW is ≥65 g/mol, the expression also depends on the wind and current velocities; the following equation is used when V_{wind} is ≤1.9 m/sec and MW is ≥65 g/mol:

$$k_1 = 23.51 \times (V_{curr}^{0.969} / Z^{0.673}) \times (32/MW)^{1/2} \text{ cm/hr} . \quad (12)$$

The following equation is used when V_{wind} is >1.9 m/sec and ≤5 m/sec, and MW is ≥65 g/mol:

$$k_1 = 23.51 \times (V_{curr}^{0.969} / Z^{0.673}) \times (32/MW)^{1/2} \, e^{0.526(V_{wind}-1.9)} \text{ cm/hr} . \quad (13)$$

No liquid-phase exchange coefficient equation is provided in Thomas (1990) for wind velocities >5 m/sec.

Combining Equations (7), (8), (9), and (11) into a single equation for estimating volatilization half-life ($\tau_{1/2}$) for compounds with MW <65 g/mol gives the following equation:

$$\tau_{1/2} = Z \times \ln 2 \times \{[(1/20) \times (MW/44)^{1/2}] + [(RT/H \times 3{,}000) \times (MW/18)^{1/2}]\} \text{ hr} . \quad (14)$$

The following equation, combining Equations (7), (8), (10), and (12), can be used to estimate the volatilization half-life ($\tau_{1/2}$) for compounds with MW ≥65 g/mol if the wind velocity is ≤1.9 m/sec:

$$\tau_{1/2} = Z \times \ln 2 \times \{[(Z^{0.673}/23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] + [(RT/H \times 1{,}137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2}]\} \text{ hr} . \quad (15)$$

The following equation, combining Equations (7), (8), (10), and (13), can be used to estimate the volatilization half-life ($\tau_{1/2}$) for compounds with MW ≥65 g/mol if the wind velocity is >1.9 m/sec and ≤5 m/sec:

$$\tau_{1/2} = Z \times \ln 2 \times \{[(Z^{0.673}/23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] \, e^{0.526(1.9-V_{wind})} + [(RT/H \times 1{,}137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2}]\} \text{ hr} . \quad (16)$$

If H is $<10^{-7}$ atm·m^3/mol, the substance is less volatile than water and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, p. 15-15) and no volatilization half-life is estimated for rivers or lakes.

3.1.1 Volatilization Half-Life for Rivers, Oceans, Coastal Tidal Waters, and the Great Lakes

In order to calculate the volatilization half-life for rivers, oceans, coastal tidal waters, and the Great Lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 5 m/sec, and the current velocity as 1 m/sec. Using these values, Equations (14) and (16) reduce to the following:

- MW <65 g/mol

$$\tau^{1/2} = 2.89 \times \{[0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (17)$$

- MW ≥65 g/mol

$$\tau^{1/2} = 2.89 \times \{[0.185 \times (MW/32)^{1/2}] + [(3.6 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (18)$$

where

H = Henry's law constant (atm·m^3/mol)
MW = Molecular weight (g/mol).

3.1.2 Volatilization Half-Life for Lakes

In order to calculate the volatilization half-life for lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec, and the current velocity as 0.05 m/sec. Using these values, Equations (14) and (15) reduce to the following:

- MW <65 g/mol

$$\tau^{1/2} = 2.89 \times \{[0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (19)$$

- MW ≥65 g/mol

$$\tau^{1/2} = 2.89 \times \{[17.2 \times (MW/32)^{1/2}] + [(3.9 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (20)$$

where

H = Henry's law constant (atm·m^3/mol)
MW = Molecular weight (g/mol).

3.2 SOIL/WATER DISTRIBUTION COEFFICIENTS (K_d)

As described in Section 2.4.5, SCDM soil/water distribution coefficients (K_d, mL/g) are based on the relationship

$$K_d = K_{oc} \times f_{oc} \quad (21)$$

where K_{oc} is the chemical's soil organic carbon/water partition coefficient (mL/g) and f_{oc} is assumed to be 0.002 g organic carbon/g soil. For organic chemicals without K_d values in SCDM datafiles SSG_KD or RTI_ION (see Section 2.4.5), SCDM calculates a K_d value based on this relationship, using a K_{oc} value calculated from a compound's SCDM Log octanol/water partition coefficient (Log K_{ow} or Log P). To perform this calculation, SCDM uses the relationship between these properties determined by DiToro (1985) for semivolatile organic compounds:

$$K_{oc} = 0.00028 + 0.983 \text{ Log } K_{ow} \text{ .} \quad (22)$$

This equation is also used in the Soil Screening Guidance (EPA, 1996b).

Combining Equations (21) and (22) yields the following equation:

$$K_d = f_{oc} \times 10^{(0.00028 + 0.983 \text{Log } K_{ow})} . \quad (23)$$

For any organic hazardous substance for which no K_d value is available in SCDM datafiles SSG_KD or RTI_ION, but with a Log K_{ow} value chosen as described in Section 2.6.2, SCDM calculates K_d using Equation (23).

3.3 SCREENING CONCENTRATION BENCHMARKS

The HRS assigns extra weight to targets with exposure levels to hazardous substances that are at or above benchmark values. In addition to the regulatory limits discussed in Section 2.8, the HRS uses a number of benchmarks called screening concentrations. Screening concentrations correspond to a 10^{-6} individual cancer risk or a noncancer hazard quotient of 1 under specified exposure assumptions. These assumptions, discussed below, are conservative and broadly apply to sites nationwide. The Agency recognizes that modeling human activity patterns would provide a more realistic determination of exposure or risk. While such information may be determined on a site-specific basis with considerable effort, it is difficult to develop assumptions on the activity patterns of target populations that could be applied to sites on a nationwide basis in order to develop exposure scenarios for the HRS. For this reason, the HRS exposure assumptions reflect values used for the assessment of risk throughout different programs within the Agency. EPA recognizes that a critical evaluation of the references cited below, along with other information, could lead to differing exposure assumptions. Moreover, the Agency is still refining the assumptions used in this area of risk assessment.

EPA also considered the limited number of samples available at the National Priority List (NPL) listing stage when it selected these assumptions. As outlined in the Field Test of the proposed revised HRS, the Agency generally expects to have <100 samples for all pathways to support the HRS analysis. This limited sampling may miss areas of maximum contamination, or "hot spots," and thus the sample results may not represent the maximum level of contamination. Although using conservative exposure assumptions does not fully compensate for the limited data available for analysis, using less conservative assumptions would likely lead to a greater incidence of false negatives; i.e., the Agency may not identify sites that should be investigated further under the remedial program.

3.3.1 Screening Concentrations for Drinking Water Pathways

The following equation (EPA, 1989b, p. 6-35) is used to calculate the average daily intake of a hazardous substance from the ingestion of contaminated ground water or surface water:

$$\text{Average Daily Intake (mg/kg–day)} = \frac{C_{water} \times IR \times EF \times ED}{BW \times AT} \qquad (24)$$

where:

C_{water} = Contaminant concentration in water (mg/L)
IR = Drinking water intake (ingestion) rate (L/day)
EF = Exposure frequency (days/year)
ED = Exposure duration (years)
BW = Body weight (kg)
AT = Averaging time (days).

Under the assumptions used for HRS purposes, the adult drinking water ingestion rate is 2 L/day, the exposure frequency for residents is daily (350 days/year), the exposure duration is 30 years, and the average adult body weight is 70 kg. The ingestion rate of 2 L/day is routinely used by the Agency as the default value for drinking water ingestion and assumes that the entire 2 L are from the contaminated drinking water source. Refinements in risk assessments sometime assume that an individual will be away for vacations or that some water will be consumed at the workplace.

Cancer Risk Screening Concentration. The cancer risk screening concentration is estimated by solving Equation (24) for the contaminant concentration in a medium of concern (C_{medium}), at a specified target risk level using the following relationship:

$$\text{Target Risk} = \text{Average Daily Intake} \times \text{Cancer Slope Factor (SF)} \; . \qquad (25)$$

When Equation (25) is rearranged to solve for the average daily intake (I), Equations (24) and (25) can be combined to estimate the water concentration (C_{water}) that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the drinking water screening concentration for carcinogens presumed to result in one excess case of cancer per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times BW \times 25{,}550 \text{ days}}{SF_{oral} \times IR \times EF \times ED} \quad . \tag{26}$$

With the exposure assumptions described above for Equation (24), Equation (26) may be simplified as:

$$SC_c \text{ (mg/L)} = \frac{8.52 \times 10^{-5}}{SF_{oral}} \quad . \tag{27}$$

This equation is used to calculate SC_c for nonradioactive carcinogenic substances. Because cancer slope factors for radionuclides are in units of pC_i^{-1}, body weight and averaging time do not apply. Thus, the following equation for radionuclides is analogous to Equation (26) for chemical carcinogens:

$$SC_c = \frac{10^{-6}}{SF_{oral} \times IR \times EF \times ED} \quad . \tag{28}$$

When the exposure assumptions described for Equation (24) are used, Equation (28) may be rewritten to estimate the concentration in water that corresponds to a target risk level of 10^{-6}. The screening concentration for radionuclides ingested in drinking water (SC_r) is given by:

$$SC_r \text{ (pC}_i\text{/L)} = \frac{4.76 \times 10^{-11}}{SF_{oral}} \quad . \tag{29}$$

Noncancer Risk Screening Concentration. The RfD is based on the assumption that thresholds exist for certain toxic effects. In general, the RfD is an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. When the acceptable daily intake for drinking water ingestion is set equal to the RfD_{oral} (i.e., hazard quotient = 1), Equation (24) may be rearranged to solve for the contaminant concentration in water that corresponds to the no adverse effects level described above. To solve for the drinking water screening concentration for noncarcinogens (SC_n), Equation (24) becomes:

$$SC_n = \frac{RfD_{oral} \times BW \times AT}{IR \times EF \times ED} \quad . \tag{30}$$

For noncarcinogenic effects, the averaging time is 30 years, or 10,950 days. When the assumptions described for Equation (24) are used, Equation (30) may be simplified as:

$$SC_n \text{ (mg/L)} = RfD_{oral} \times 36.5 \quad . \tag{31}$$

3.3.2 Screening Concentrations for the Surface Water Food Chain Pathway

The following equation (EPA, 1989b, p. 6-45) is used to calculate the average daily intake from fish and shellfish ingestion:

$$\text{Average Daily Intake (mg/kg-day)} = \frac{C_{fish} \times IR \times F \times EF \times ED}{BW \times AT} \tag{32}$$

where:

C_{fish} = Contaminant concentration in fish/shellfish (mg/kg)
IR = Fish/shellfish intake (ingestion) rate (kg/day)
F = Fraction ingested from contaminated source (unitless)
EF = Exposure frequency (days/year)
ED = Exposure duration (years)
BW = Body weight (kg)
AT = Averaging time (days).

The high end fish ingestion rate for recreational fishers is 0.054 kg/day (USDA, 1982), with the fraction ingested (F) set equal to 1 (i.e., all fish are assumed to come from contaminated waters). The exposure frequency is assumed to be 350 days/year, the exposure duration is 30 years, and the average adult body weight is 70 kg.

Cancer Risk Screening Concentration. When Equation (25) is rearranged to solve for the average daily intake (I), Equations (25) and (32) can be combined to estimate the fish/shellfish concentration that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for

carcinogenic effects. Therefore, the fish/shellfish concentration presumed to result in one excess case of cancer per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times BW \times 25{,}550 \text{ days}}{SF_{oral} \times IR \times F \times EF \times ED} \quad . \tag{33}$$

Using the exposure assumptions listed for Equation (31) results in a simplified screening concentration equation for nonradioactive carcinogenic substances in fish/shellfish:

$$SC_c \text{ (mg/kg)} = \frac{3.15 \times 10^{-3}}{SF_{oral}} \quad . \tag{34}$$

If the same exposure assumptions, excluding body weight and averaging time, are used, Equation (34) may be rewritten to estimate the fish/shellfish concentration that corresponds to a target risk level of 10^{-6} for ingestion of radionuclides in fish and shellfish (SC_r):

$$SC_r \text{ (pC}_i\text{/kg)} = \frac{1.76 \times 10^{-9}}{SF_{oral}} \quad . \tag{35}$$

Noncancer Risk Screening Concentration. Setting the intake from fish and shellfish ingestion equal to the oral reference dose (RfD_{oral}) and solving Equation (32) for concentration gives the following equation:

$$SC_n = \frac{RfD_{oral} \times BW \times AT}{IR \times F \times EF \times ED} \quad . \tag{36}$$

For noncarcinogenic effects, the averaging time is 30 years, or 10,950 days. If the other assumptions listed for Equation (32) are used, Equation (36) may be simplified as follows:

$$SC_n \text{ (mg/kg)} = RfD_{oral} \times 1{,}352 \quad . \tag{37}$$

3.3.3 Screening Concentrations for Soil Ingestion

The following equation (EPA, 1991, p. 3-25) is used to calculate the average daily intake from soil ingestion:

$$\text{Average Daily Intake (mg/kg-day)} = \frac{C_{soil} \times CF \times IF \times EF}{AT} \quad (38)$$

where:

C_{soil} = Contaminant concentration in soil (mg/kg)
CF = Conversion factor (10^{-6} kg/mg)
IF = Age-adjusted soil ingestion factor (mg-yr/kg-day)
EF = Exposure frequency (days/year)
AT = Averaging time (days)

and IF is given by:

$$IF_{soil/adj}\ \text{(mg-yr/kg-day)} = \frac{IR_{soil/age1-6} \times ED_{age1-6}}{BW_{age1-6}} + \frac{IR_{soil/age7-13} \times ED_{age7-31}}{BW_{age7-31}} \quad (39)$$

where:

$IR_{soil/age1-6}$ = Soil intake (ingestion) rate, age 1 to 6 (mg/day)
ED_{age1-6} = Exposure duration during ages 1-6 (yr)
BW_{age1-6} = Average body weight from ages 1-6 (kg)
$IR_{soil/age7-31}$ = Soil intake (ingestion) rate, ages 7 and older (mg/day)
$ED_{age7-31}$ = Exposure duration during ages 7-31 (yr)
$BW_{age7-31}$ = Average body weight from ages 7-31 (kg).

The soil ingestion rate is assumed to be 200 mg/day for ages 6 and younger, and 100 mg/day for ages 7 and older; the exposure durations are 6 years and 24 years for children and "adults" (ages 7 to 31), respectively; and the average body weights are 15 kg for children and 70 kg for adults. As with Equation (24), the exposure frequency is assumed to be 350 days/year. With these assumptions, the age-adjusted soil ingestion factor is 114 mg-yr/kg-day.

Cancer Risk Screening Concentration. When Equation (25) is rearranged to solve for the average daily intake (I), Equations (25) and (38) can be combined to estimate the soil concentration that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the screening soil concentration presumed to result in one excess case of cancer per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times 25{,}500 \text{ days}}{SF_{oral} \times IF \times CF \times EF} . \quad (40)$$

Using the assumptions listed for Equations (38) and (39) results in a simplified screening concentration equation for nonradioactive carcinogenic substances in soil:

$$SC_c \text{ (mg/kg)} = \frac{0.640}{SF_{oral}} . \quad (41)$$

Since cancer slope factors for radionuclides are provided in pCi^{-1}, body weight and averaging time do not apply. As a result, IF is calculated without body weight (BW) in Equation (39) and is equal to 3,600 mg-yr/day. If the other exposure assumptions described for chemical carcinogens are used, Equation (41) may be rewritten to estimate the soil concentration that corresponds to a target risk level of 10^{-6} for ingestion of radionuclides in contaminated soils (SC_r):

$$SC_r \text{ (pC}_i\text{/kg)} = \frac{7.94 \times 10^{-7}}{SF_{oral}} . \quad (42)$$

Noncancer Risk Screening Concentration. Setting the intake from soil ingestion equal to the oral reference dose (RfD_{oral}) and solving Equation (38) for concentration gives the following equation:

$$SC_n = \frac{RfD_{oral} \times BW \times AT}{IR \times CF \times EF \times ED} . \quad (43)$$

For noncarcinogenic effects, the averaging time (AT) is a function of the exposure duration (ED) assumed for children or 6 years × 365 days/year = 2,190 days. Assuming daily exposure (i.e., EF = 350 days/year), an average body weight of 15 kg, and an ingestion rate (IR) for children of 200 mg soil per day results in the following simplified equation:

$$SC_n \text{ (mg/kg)} = RfD_{oral} \text{ (mg/kg-day)} \times 78{,}214 \ . \qquad (44)$$

3.3.4 Screening Concentrations for the Air Pathway

The following equation (EPA, 1989b, p. 6-44) is used to calculate intake from inhalation of airborne hazardous substances:

$$\text{Average Daily Intake (mg/kg-day)} = \frac{C_{air} \times IR \times EF \times ED}{BW \times AT} \qquad (45)$$

where:

C_{air} = Contaminant concentration in air (mg/m^3)
IR = Air intake (inhalation) rate (m^3/day)
EF = Exposure frequency (days/year)
ED = Exposure duration (years)
BW = Body weight (kg)
AT = Averaging time (days).

The inhalation rate is assumed to be 20 m^3/day, the exposure frequency is 350 days/year, the exposure duration is 30 years, and the average adult body weight is 70 kg.

Cancer Risk Screening Concentration. By rearranging Equation (25) to solve for the average daily intake (I), Equations (25) and (45) can be combined to estimate the concentration in air that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the air concentration presumed to result in one excess case of cancer per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times BW \times 25{,}550 \text{ days}}{SF_{inhal} \times IR \times EF \times ED} \ . \qquad (46)$$

Using the exposure assumptions listed above for Equation (45) results in the following equation for nonradioactive carcinogenic substances:

$$SC_c\ (mg/m^3) = \frac{8.52 \times 10^{-6}}{SF_{inhal}}\ . \qquad (47)$$

Using the same exposure assumptions (excluding body weight and averaging time), Equation (46) may be rewritten to estimate the air concentration of radionuclides that corresponds to a target risk level of 10^{-6} for inhalation of contaminated air (SC_r):

$$SC_r\ (pC_i/m^3) = \frac{4.76 \times 10^{-12}}{SF_{inhal}}\ . \qquad (48)$$

Noncancer Risk Screening Concentration. Setting the average daily intake equal to the inhalation reference dose (RfD_{inhal}) and solving Equation (45) for the air concentration results in the following equation:

$$SC_n = \frac{RfD_{inhal} \times BW \times AT}{IR \times EF \times ED}\ . \qquad (49)$$

For noncarcinogenic effects, the averaging time (AT) is 30 years, or 10,950 days. The inhalation rate (IR) is assumed to be 20 m^3/day, the exposure frequency (EF) is 350 days/year, the exposure duration (ED) is 30 years, and the average adult body weight (BW) is 70 kg. When these assumptions are used, Equation (49) may be simplified as:

$$SC_n\ (mg/m^3) = RfD_{inhal} \times 3.65\ . \qquad (50)$$

SECTION 4

CHEMICAL DATA, FACTOR VALUES, AND BENCHMARKS

Appendix A contains a two-page listing of selected data, HRS factor values, and benchmarks for each hazardous substance in SCDM (the "SCDM page reports"). Data selected for SCDM for each substance are on the first page; factor values and benchmarks are on the second page.

Figure 1 presents the header that appears on both sides of the page report. The header contains the date the report was printed, the substance name and synonym, the SCDM version (month, year), and the Chemical Abstract Service (CAS) number for the substance.

```
Date:      06/15/96                SUPERFUND CHEMICAL DATA MATRIX          SCDM Version: JUN96
Chemical:  Acenaphthene                                                    CAS Number:   000083-32-9
```

Figure 1. Page Heading

The first page contains all of the selected chemical data, the data units, and an acroynym describing the source of the information in SCDM. The chemical data are divided into six functional groups: toxicity, persistence, physical characteristics, mobility, bioaccumulation, and other data.

The toxicity section (Figure 2) contains the acute, chronic, and carcinogenicity data that were compiled using the methodology described in Sections 2.2, 2.3, and 2.7 and used to derive toxicity and ecotoxicity factor values. The top half of this section contains the data used to determine the human toxicity factor value: reference dose (oral and inhalation), cancer slope factor (oral and inhalation), ED_{10} (oral and inhalation),

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	6.0E-02	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh AWQC:		µg/L	
Salt AWQC:		µg/L	
Fresh AALAC:		µg/L	
Salt AALAC:		µg/L	
CHRONIC			
Fresh AWQC:		µg/L	
Salt AWQC:		µg/L	
Fresh AALAC:		µg/L	
Salt AALAC:		µg/L	
Fresh Ecol LC50:	6.0E+01	µg/L	AQUIRE
Salt Ecol LC50:	2.2E+03	µg/L	AQUIRE

Figure 2. Toxicity Section

LD_{50} (oral and dermal), and LC_{50} (gas and dust inhalation). The bottom half of this section contains the data used to determine an ecotoxicity factor value: acute and chronic ambient water quality criteria (AWQC) for fresh and salt water, acute and chronic aquatic life advisory concentrations (AALACs) for fresh and salt water (at this time no AALACs have been promulgated), and fresh and salt water LC_{50} values. Blank entries indicate that no value was found using the procedures and references specified in Section 2.

The persistence section (Figure 3) contains the surface water persistence data compiled using the methodology described in Sections 2.5, 2.6.2, and 3.1. Surface water persistence factors can also be determined using the logarithm of the *n*-octanol/water partition coefficient (Log K_{ow} or Log P) if, as specified in the HRS, this gives a higher factor value than the half-lives (or a default, if applicable).

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.1E+02	days	THOMAS
Photolysis:	2.5E+00	days	FATERATE
Biodeg:	1.0E+02	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.4E+00	days	THOMAS
Photolysis:	2.5E+00	days	FATERATE
Biodeg:	1.0E+02	days	FATERATE
Radio:		days	
Log Kow:	3.9E+00		RTI_LOGP

Figure 3. Persistence Section

The physical characteristics section (Figure 4) contains logical "yes/no" flags that classify the substance. The "metal contain" flag indicates that the hazardous substance is a metal or metalloid and is used to determine ground water mobility and surface water persistence factors. The "organic" and "inorganic" flags are used to determine ground water mobility and bioaccumulation. The "radionuclide" flag is used to determine the human toxicity factor, the ecosystem toxicity factor, and the surface water persistence factor. The radioactive element flag ("rad. element") is used to determine whether or not the HRS factors and benchmarks (second page) are printed. The gas and particulate flags are used to determine mobility and likelihood of release for the air pathway. Molecular weight is used to determine volatilization half-life, as described in Section 3.1.

PHYSICAL CHARACTERISTICS

Parameter	Value
Metal Contain:	No
Organic:	Yes
Inorganic:	No
Gas:	Yes
Particulate:	Yes
Radionuclide:	No
Rad. Element:	No
Molecular Weight:	1.5E+02
Density:	1.0E+00 g/mL @ 99.00° C

Figure 4. Physical Characteristics

The mobility section (Figure 5) contains the air and ground water mobility data compiled using the methodology described in Sections 2.4.3, 2.4.4, 2.4.5, and 3.2. Vapor pressure and

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.5E-03	Torr	CHEMFATE
Henry's Law:	1.6E-04	atm-m3/mol	CHEMFATE
Water Solub:	4.2E+00	mg/L	LIVECHEM
Distrib Coef:	1.4E+01	ml/g	
Geo. Mean Sol.:			

Figure 5. Mobility Section

Henry's law constant are used to determine gas migration potential and gas mobility factors. Henry's law constant is also used to calculate the volatilization half-life as described in Section 3.1. Water solubility and the soil/water distribution coefficient are used to determine the ground water mobility factor. Substance-specific water solubility is used for nonmetal and nonmetalloid substances, whereas for metal-containing substances the solubility value is the geometric mean of the available water solubilities for inorganic compounds containing the hazardous substance.

The bioaccumulation section (Figure 6) contains the human food chain and environmental bioaccumulation potential factor data compiled using the methodology described in Section 2.6. Bioconcentration factors (BCFs) are collected for fresh and salt water for the human food chain and environmental threats. Log K_{ow} or water solubility is used to establish bioaccumulation potential when a BCF is not available.

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	3.9E+02		VER_BCF
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	3.9E+02		VER_BCF
Salt BCF:			
Log Kow:	3.9E+00		RTI_LOGP
Water Solub:	4.2E+00	mg/L	LIVECHEM

Figure 6. Bioaccumulation Section

The section labeled "other data" (Figure 7) contains values for melting points and boiling points (°C) along with the associated vapor pressure (Torr), if applicable. Chemical formula is also listed here.

OTHER DATA

Melting Point :93.40° C
Boiling Point :279.00° C
Formula :C12H10

Figure 7. Other Data Section

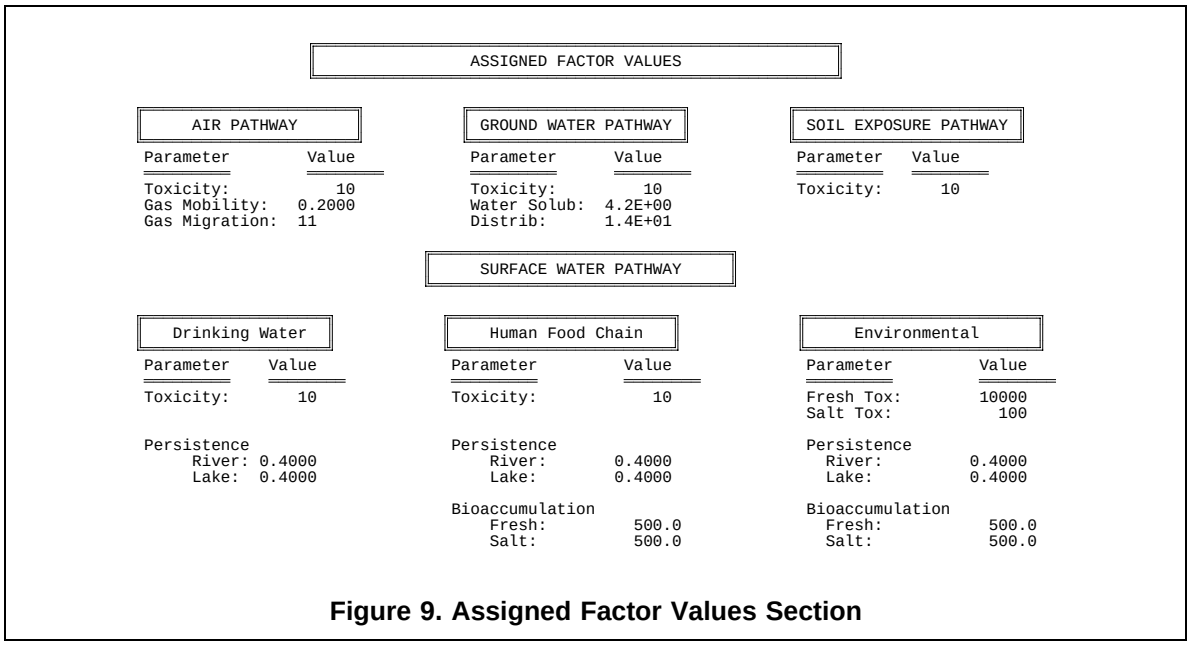
The class information section (Figure 8) lists parent substances for three data substitution classes: toxicity, ground water mobility, and other data. The toxicity class includes all toxicity and benchmark data used to determine human or ecotoxicity factor values. The ground water mobility class includes water solubility, soil/water distribution coefficient, and geometric mean water solubility. The "other" class includes hydrolysis, biodegradation, photolysis, and volatilization half-lives, as well as BCFs and Log K_{ow}.

CLASS INFORMATION

Class	Parent Substance
Toxicity:	NA
GW Mob:	NA
Other:	NA

Figure 8. Class Information Section

Currently only two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for the ground water mobility class with the elemental metal as the class parent. Radioactive isotopes may inherit data from their primary radioactive element for the ground water mobility and "other" classes.



ASSIGNED FACTOR VALUES

AIR PATHWAY

Parameter	Value
Toxicity:	10
Gas Mobility:	0.2000
Gas Migration:	11

GROUND WATER PATHWAY

Parameter	Value
Toxicity:	10
Water Solub:	4.2E+00
Distrib:	1.4E+01

SOIL EXPOSURE PATHWAY

Parameter	Value
Toxicity:	10

SURFACE WATER PATHWAY

Drinking Water

Parameter	Value
Toxicity:	10
Persistence	
River:	0.4000
Lake:	0.4000

Human Food Chain

Parameter	Value
Toxicity:	10
Persistence	
River:	0.4000
Lake:	0.4000
Bioaccumulation	
Fresh:	500.0
Salt:	500.0

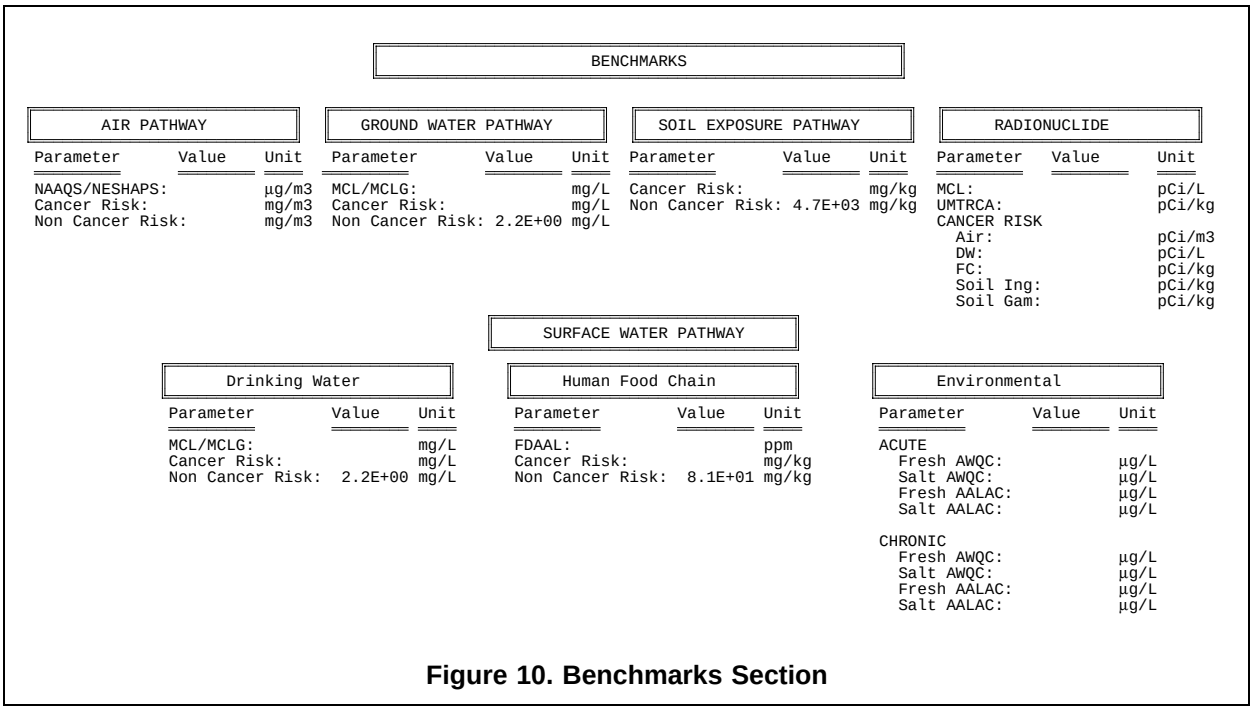
Environmental

Parameter	Value
Fresh Tox:	10000
Salt Tox:	100
Persistence	
River:	0.4000
Lake:	0.4000
Bioaccumulation	
Fresh:	500.0
Salt:	500.0

Figure 9. Assigned Factor Values Section

The second page for each substance is divided into top and bottom sections that contain factor values (Figure 9) and benchmarks (Figure 10) required by the HRS. SCDM determines factor values using HRS methodologies, from selected data on the first page of the SCDM page report. The factor values are presented by pathway: air, ground water, soil exposure, and surface water. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. The toxicity factor value represents human toxicity and is the same for all pathways. The air pathway gas migration factor value is used to determine likelihood of release. The surface water environmental toxicity factor values are based on fresh and salt water ecosystem toxicity data, and the surface water persistence factor values are based on BCFs for all aquatic species. The surface water human food chain factor values are based on human toxicity and BCFs for only those aquatic species consumed by humans. For radioactive substances, human toxicity, ecosystem toxicity, and surface water persistence factor values are determined as specified in Chapter 7 of the HRS.

The benchmarks (Figure 10), like the factor values, are presented by pathway: air, ground water, soil exposure, and surface water. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. For HRS scoring, actual sampled contaminant concentrations for a particular media are compared to these benchmark concentrations to determine if the target will be scored as subject to Level I or Level II contamination.



BENCHMARKS

AIR PATHWAY

Parameter	Value	Unit
NAAQS/NESHAPS:		µg/m3
Cancer Risk:		mg/m3
Non Cancer Risk:		mg/m3

GROUND WATER PATHWAY

Parameter	Value	Unit
MCL/MCLG:		mg/L
Cancer Risk:		mg/L
Non Cancer Risk:	2.2E+00	mg/L

SOIL EXPOSURE PATHWAY

Parameter	Value	Unit
Cancer Risk:		mg/kg
Non Cancer Risk:	4.7E+03	mg/kg

RADIONUCLIDE

Parameter	Value	Unit
MCL:		pCi/L
UMTRCA:		pCi/kg
CANCER RISK		
Air:		pCi/m3
DW:		pCi/L
FC:		pCi/kg
Soil Ing:		pCi/kg
Soil Gam:		pCi/kg

SURFACE WATER PATHWAY

Drinking Water

Parameter	Value	Unit
MCL/MCLG:		mg/L
Cancer Risk:		mg/L
Non Cancer Risk:	2.2E+00	mg/L

Human Food Chain

Parameter	Value	Unit
FDAAL:		ppm
Cancer Risk:		mg/kg
Non Cancer Risk:	8.1E+01	mg/kg

Environmental

Parameter	Value	Unit
ACUTE		
Fresh AWQC:		µg/L
Salt AWQC:		µg/L
Fresh AALAC:		µg/L
Salt AALAC:		µg/L
CHRONIC		
Fresh AWQC:		µg/L
Salt AWQC:		µg/L
Fresh AALAC:		µg/L
Salt AALAC:		µg/L

Figure 10. Benchmarks Section

Appendix B-1 contains tables for nonradioactive hazardous substances. The first table in Appendix B-1 lists all of the factor values by pathway. The second table presents the benchmarks for the air and ground water pathways, the third table presents benchmarks for the surface water pathway, and the fourth table presents benchmarks for the soil exposure pathway. Appendix B-2 contains tables for radionuclides; the first table lists all of the factor values by pathway, and the second table presents benchmarks for all pathways. Appendix C contains a cross-reference index of hazardous substance names, synonyms, and CAS numbers for substances in SCDM.

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